Comment on the papers ‘Creep and recrystallization of large polycrystalline masses’ by Faria and co-authors

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In a series of three papers, Faria and co-authors have presented the application of the theory of mixture with continuous diversity to the creep and recrystallization processes of large polycrystalline masses. In this approach, a material point of the continuum is composed of a huge number of grains defined by their crystallographic orientation. The polycrystal is then seen as a continuous mixture of lattice orientations. All the balance equations are expressed to describe the response of the polycrystal and of a group of crystallites sharing the same lattice orientation (i.e. a species). To go further, Faria and co-authors have to make the hypothesis that the strain rate of every species is equal to the strain rate of the polycrystal, and is therefore independent of its lattice orientation. Furthermore, Faria and co-authors insist on the fact that this hypothesis is negligible and has no relation at all to any kind of Taylor-type constraint on the deformation of individual grains, arguing that in their theory of strain rate inhomogeneities on the grain level are smeared out because each species is composed of a very large number of crystals. In this comment, I show that the results obtained with a full-field model suggest that this hypothesis is not insignificant.

Keywords: polycrystal; anisotropy; ice; full-field models

In a series of three papers (Faria 2006a, b; Faria et al. 2006), Faria and co-authors have presented the fundamentals of the so-called theory of mixture with continuous diversity applied to the creep and recrystallization processes of large polycrystalline masses. The third paper (Faria 2006b) is dedicated to some applications of the theory to large ice sheets. In this theory, a material particle of the continuum is composed of a huge number of grains defined by their orientations, denoted as c in what follows. Grains with the same orientation c belong to the same species.

To clarify the following discussion, the per-species (or per-phase, defined over grains having the same orientation c) averages of a quantity $y$ is defined via $Y^* = \langle y \rangle^*$, where $y$ is the quantity for a grain and $\langle \cdot \rangle^*$ denotes the per-species average. The macroscopic (polycrystal) equivalent quantity follows as $Y = \langle Y^* \rangle = \langle \langle y \rangle^* \rangle$, where $\langle \cdot \rangle$ denotes the average over all the orientations of a...
per-phase averaged quantity. More precisely, the mechanical fields are generally heterogeneous inside grains so that $y$ should be seen as the average value for a particular grain of the corresponding field inside this grain. Note that the grain quantity $y$ and so the corresponding field inside grains are never used in the theory of Faria and co-authors.

In most common cases, and particularly in the third paper (Faria 2006b) where some applications are presented, Faria and co-authors have to make the so-called assumption of negligible grain shifting (see remark 3.5 in Faria (2006a)), which provides a prodigious simplification to the theory. This assumption is that the strain rate of every species $D^*$ is equal to the strain rate of the polycrystal $D$, i.e. $D^* = \langle d \rangle^* = D$, where $d$ is the strain rate for a grain. Faria and co-authors argue that this assumption is negligible because in the present theory stress and strain inhomogeneities on the grain level are smeared out and the average response of the grains belonging to a given species does not depend any more on the species orientation (see footnote 11 in Faria (2006a)). According to Faria, all crystallites may undergo arbitrary deformations, but the orientation independence of the per-species averaged strain rate arises because each species is composed of a very large number of crystals.

In recent papers, Lebensohn and colleagues were able to evaluate, using full-field models, the strain rate and stress inhomogeneities developing during the plastic deformation of a polycrystal. Such models solve properly the Stokes equations using either a classical finite element method (FE; Lebensohn et al. 2003) or fast Fourier transforms (FFTs; Lebensohn et al. 2004a, b). This later performs better than an FE calculation for the same purpose and resolution, but only works for periodic boundary conditions. In these approaches, each crystal is decomposed into many elements, allowing one to infer the stress and strain rate heterogeneities at the microscopic scale. The deviation from the average of stress and strain rate in a particular grain depends both on the grain orientation, $c$, and on the orientations of neighbouring grains.

As an important result these models show that, for a given orientation $c$, the strain rate, $d$, and stress, $s$, for a grain are strongly dependent on the neighbour grain orientations and a high dispersion is found for $d$ and $s$ of grains having the same orientation $c$ (Lebensohn et al. 2003). On the other hand, the per-species average values $D^* = \langle d \rangle^*$ and $S^* = \langle s \rangle^*$ are still dependent on the species orientation $c$ (Lebensohn et al. 2004a). In other words, the neighbourhood influence does not counteract the orientation influence of the average behaviour of a large number of grains having the same orientation. Owing to the neighbourhood influence, the dispersion of the strain rate and stress of the grains with the same orientation can be very large, but the per-species averaged strain rate and stress are definitively not equal to the macroscopic strain rate and stress, respectively, but follow an orientation-dependent function: $S^* = S^*(c) \neq S$ and $D^* = D^*(c) \neq D$.

While the theory of mixture with continuous diversity deals with a huge number of grains, full-field models contain only a limited number of grains. Could it be that, for a given fabric (a given second-order orientation tensor, for example), increasing the number of grains would decrease the orientation dependency of $S^*$ and $D^*$? Lebensohn et al. (2004a) have studied the dependency to the number of grains of the per-species averaged stress and strain rate. Their results indicate (see fig. 2 in Lebensohn et al. (2004a)) that for a small number of grains (few different neighbours’ configurations for a given orientation), the response of a species is influenced as much
by its neighbours’ orientations as by its own orientation. For a large number of grains, the influences of the different neighbours’ configuration are then averaged out, and the species response is mainly dictated by its orientation. Increasing the number of grains induces only a decrease in the neighbours’ influence but, on no account, the species response is equal to the macroscopic one and independent of its orientation.

Moreover, Faria and co-authors emphasize the fact that the negligible grain shifting hypothesis has no relation at all to any kind of Taylor-type constraint on the deformation of individual grains (see footnote 11 in Faria (2006a) and remark 2.1 and third paragraph of the conclusion in Faria (2006b)). Effectively, the negligible grain shifting hypothesis does not imply that the strain rate of each grain is equal to the strain rate of the polycrystal. In the theory of mixture with continuous diversity, the average strain rate, \( \mathbf{d} \), of each grain is never inferred, and all the equations are written in terms of the per-species averaged strain rates, \( \mathbf{D}^* \), or the polycrystal strain rates, \( \mathbf{D} \). As a consequence, a polycrystal law derived from the theory is implicitly built assuming an orientation-independent strain rate, as shown by eqn (3.3)_II \( (S'_{ij} = \mu^*_{ijkl} D_{kl}) \) in Faria (2006b), resulting in an expression for the stress equivalent to that one obtained using a Taylor-type assumption in the framework of the homogenization model.

The FFT results in Lebensohn et al. (2004a) clearly contradicting the statement made by Faria and co-authors that stress and strain rate of a species should be independent of its orientation owing to the huge number of grains belonging to the same species. The assumption made by Faria and others is not insignificant and is comparable to a uniform strain rate or Taylor-type assumption in the framework of the homogenization model. As shown by Castelnau et al. (1996), for a strongly anisotropic material like ice, the uniform strain rate assumption is really not appropriate and it would be better, at least, to adopt the uniform stress assumption. This will have to be discussed in the coming papers using the theory of mixture with continuous diversity.

References


